Fermi Surface and gap parameter in high- T_c superconductors: the Stripe Quantum Critical Point scenario

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Abstract

We study the single-particle spectral properties of electrons coupled to quasicritical charge and spin fluctuations close to a stripe-phase, which is governed by a Quantum Critical Point near optimum doping. We find that spectral weight is transferred from the quasiparticle peak to incoherent dispersive features. As a consequence the distribution of low-laying spectral weight is modified with respect to the quasiparticle Fermi surface. The interplay of charge and spin fluctuations reproduces features of the observed Fermi surface, such as the asymmetric suppression of spectral weight near the M points of the Brillouin zone.

Within the model, we also analyze the interplay between repulsive spin and attractive charge fluctuations in determining the symmetry and the peculiar momentum dependence of the superconducting gap parameter. When both spin and charge fluctuations are coupled to the electrons, we find $d_{x^2-y^2}$ -wave gap symmetry in a wide range of parameter. A crossover d- vs s-wave symmetry of the gap may occur when the strength of charge fluctuations increases with respect to spin fluctuations.

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I. INTRODUCTION

A few theories for high- T_c cuprate superconductors are based on the presence of a Quantum Critical Point (QCP) of some kind of instability in the phase diagram of these materials.

The different realizations of this scenario proposed so far involve (i) an antiferromagnetic (AFM)-QCP [1,2], (ii) a charge-transfer instability [3], (iii) an "as-yet unidentified" QCP regulating a first-order phase-transition between the AFM state and the superconducting SC state [4], (iv) an incommensurate charge-density-wave (ICDW)-QCP [5,6].

The theories based on the AFM-QCP [1,2] are motivated by the presence of an AFMphase at low doping and by the observation of strong spin fluctuations at larger doping [7–10]. However near and above optimum doping it is likely that charge degrees of freedom play a major role, whereas spin degrees of freedom follow the charge dynamics, and are enslaved by the charge instability controlled by the ICDW-QCP [5,6,11], as suggested also by the experiments in $La_{2-x}(NdSr)_xCuO_4$ [12]. The strong interplay between charge and spin degrees of freedom extends the spin fluctuations to a region far away from the AFM-QCP and gives rise to a "stripe phase" which continuously connects the onset of the charge instability (ICDW-QCP) at high doping with the low-doping regime, where mobile holes, expelled by the AFM background, may form fluctuating stripes with marked one dimensional character [13]. Thus, we shall more properly refer to the ICDW-QCP as the Stripe-QCP. The AFM-QCP and the Stripe-QCP are not alternative and they control the behaviour of the system in different regions of doping. On the other hand the existence of a Stripe-QCP at optimum doping, where no other energy scale besides the temperature is present in transport measurements [14], is the natural explanation for the peculiar nature of this doping regime in the phase diagram of superconducting copper oxides. Indeed the critical fluctuations near a QCP provide a singular electron-electron (e-e) interaction which may account for both the violation of the Fermi liquid (FL) behaviour in the metallic state and the high superconducting critical temperature [5,6].

In this paper we focus on the outcomes of the Stripe-QCP scenario with respect to

the single particle excitation spectra in the normal state and the symmetry of the gap parameter in the superconducting state and we compare our results with the corresponding experiments, as discussed below.

The angle-resolved photoemission spectroscopy (ARPES), mainly performed on $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212), is providing new evidence for an anomalous metallic state in the under- and optimally doped region of the phase diagram of high- T_c cuprate superconductors. The single-particle excitation spectra show features which cannot be described within the conventional Fermi liquid theory. The underdoped region is characterized by the opening of a pseudogap around the M points of the Brillouin zone (BZ) below a crossover temperature T^* , which seems to evolve into the superconducting gap at the critical temperature T_c [15–17]. At the same time and in the same region of the BZ, the quasiparticle peaks in the energy distribution curves have a rather low spectral intensity and are very broad, even near the leading edge. At optimum doping, where the pseudogap disappears, a strong suppression of low-laying spectral weight around the M points is still present [16,18]. Furthermore, the recently developed angular scanning photoemission spectroscopy provides a detailed picture of the k-space distribution of spectral weight near the Fermi level and shows that the suppression around the M points is asymmetric [18]. The energy distribution curves are characterized by the presence of dispersive peaks of incoherent nature besides the quasiparticle peak |16|.

In the superconducting state, the gap parameter has a peculiar doping and temperature dependence. In the under- and optimally doped region of the phase diagram, ARPES measurements on Bi2212 [19] and on $YBa_2Cu_3O_{7-\delta}$ (Y123) [20] have shown that the magnitude of the superconducting gap parameter is strongly momentum dependent in agreement with a $d_{x^2-y^2}$ -wave or a strongly anisotropic s-wave gap. Several phase-sensitive measurements on Y123, involving currents flowing within the CuO_2 planes [21–23], together with temperature dependent penetration depth measurements [24], provide evidence for primarily $d_{x^2-y^2}$ -wave gap. On the other hand c-axis Josephson tunneling experiments, and in particular the measurements where a conventional s-wave superconductor (Pb) is deposited across a single twin

boundary of Y123 twinned crystal, show that the gap has a sizeable s-wave component [25].

In overdoped Bi2212 ARPES experiments, out of the experimental error, detect a finite value of the gap [26,27], hence the gap cannot have d-wave symmetry. The measured anisotropic ratio $r = \Delta_{max}/\Delta_{min}$ is a decreasing function of the doping, having $r \simeq 20$ near optimal doping, compatible with d-wave gap, and $r \simeq 1.5$ at overdoping, compatible with anisotropic s-wave gap. In the same range of doping, the topology of the FS, including the saddle points, does not change significantly [27]. We take this as an indication that the strong doping dependence of the gap parameter comes from a corresponding strong doping dependence of the e-e effective interaction.

II. THE NORMAL STATE

We study the single-particle excitation spectra of the metallic phase in the vicinity of the Stripe-QCP. The charge (c) and (enslaved) spin (s) fluctuations near the QCP, mediate an effective electron-electron interaction, which in the random phase approximation can be written as

$$\Gamma_{eff}(q,\Omega) = \Gamma_c(q,\Omega) + \Gamma_s(q,\Omega) = -\sum_{i=c,s} \frac{V_i}{\kappa_i^2 + \omega_i^2(q) - i\gamma_i\Omega},$$
(1)

where γ_i is a damping coefficient and $\omega_i^2(q) = 2[2 - \cos(q_x - q_x^i) - \cos(q_y - q_y^i)]$ is taken in the cos-like form to reproduce the $(q - q^i)^2$ behaviour close to the wave-vector $q^i \equiv (q_x^i, q_y^i)$ of the critical charge and spin fluctuations, and to maintain the lattice periodicity near the zone boundary. The distance from criticality is measured by the inverse squared of the correlation length $\kappa_i^2 \sim \max[a(\delta - \delta_c), bT]$; we locate the Stripe-QCP at a hole doping $\delta_c \simeq \delta_{optimal}$. The form (1) for the effective interaction, mediated by charge fluctuations, was found within a slave-boson approach to the Hubbard-Holstein model with long-range Coulomb interaction, close to the charge instability [5,28]. The same form, mediated by spin fluctuations, corresponds to the phenomenological susceptibility proposed in Ref. [29] to fit NMR and neutron scattering experiments, in the strongly damped limit. The condition that

charge fluctuations enslave spin fluctuations near the Stripe-QCP is introduced, within our model, by requiring that the vanishing of κ_c^2 drives κ_s^2 to zero.

The bare electron dispersion law is taken in the form

$$\xi(k) = -2t(\cos k_x + \cos k_y) + 4t'\cos k_x \cos k_y - \mu, \tag{2}$$

where nearest-neighbour (t) and next-to-nearest-neighbour (t') hopping terms are considered, to reproduce the main features of the band dispersion and the FS observed in high- T_c materials. We choose t=200 meV, t'=50 meV, and $\mu=-180$ meV, corresponding to a hole doping $\delta \simeq 0.17$ with respect to half filling, as appropriate for Bi2212 at optimal doping.

Aiming to capture the essential aspects of the single-particle excitation spectra, we calculate the electron self-energy within perturbation theory, considering the first-order contribution $\Sigma(k,\varepsilon) = \Sigma_c(k,\varepsilon) + \Sigma_s(k,\varepsilon)$. The imaginary part of the self-energy is

$$Im\Sigma(k,\varepsilon) = \sum_{i=c,s} V_i \gamma_i^{-1} \int_{BZ} \frac{dk_x' dk_y'}{4\pi^2} \frac{[f(\xi(k')) + b(\xi(k') - \varepsilon)] [\varepsilon - \xi(k')]}{[\varepsilon - \xi(k')]^2 + \gamma_i^{-2} [\kappa_i^2 + \omega_i^2 (k - k')]^2},$$
 (3)

where the integral is extended over the BZ, $f(\varepsilon)$ is the Fermi function and $b(\varepsilon)$ is the Bose function. The real part of the self-energy $\text{Re}\Sigma(k,\varepsilon)$ is obtained by a Kramers-Krönig transformation of (3). To preserve the inversion symmetry $k\to -k$ in the resulting quasiparticle spectra, we symmetrize the self-energies $\Sigma_{c,s}$ with respect to $\pm q^{c,s}$. For the sake of simplicity we assume that $q^s=(\pi,\pi)$, neglecting the possibility for a discommensuration of the spin fluctuations in a (dynamical) stripe phase [12], which would introduce minor changes to the resulting self-energy. The direction and the magnitude of the critical wave-vector q^c are not universal. They depend on both the material [30] and the model [31,13]. To discuss the ARPES experiments, which are mainly performed on Bi2212 samples, we consider this material and we take $q^c=(0.4\pi, -0.4\pi)$ as it is suggested by the analysis of the experimental results [18]. The other parameters appearing in the effective interaction (1) are taken as $V_{c,s}=0.4$ eV, $\kappa_{c,s}^2=0.01$ and $\gamma_{c,s}=10$ eV⁻¹. We focus on the quantum critical region near optimal doping, where the only energy scale is the temperature ($\kappa_{c,s}^2 \sim T$) and a strong violation of the Fermi-liquid behaviour in the metallic phase is found.

To study the effect of the singular interaction (1) on the single-particle properties in the metallic phase we calculate the spectral density $A(k,\varepsilon) = \pi^{-1}|\mathrm{Im}\Sigma(k,\varepsilon)|/\{[\varepsilon - \xi(k) + \mu' - \mathrm{Re}\Sigma(k,\varepsilon)]^2 + [\mathrm{Im}\Sigma(k,\varepsilon)]^2\}$. The chemical potential is self-consistently corrected by a term μ' to keep the number of particles fixed. To simulate the experimental conditions in ARPES measurements we introduce the convoluted spectral density

$$\tilde{A}_R(k,\varepsilon) = \int_{-\infty}^{+\infty} d\varepsilon' A(k,\varepsilon') f(\varepsilon') E_R(\varepsilon' - \varepsilon), \tag{4}$$

which takes care of the absence of occupied states above the Fermi energy, through the Fermi function $f(\varepsilon)$, and of the experimental energy resolution R, through a resolution function $E_R(\varepsilon)$. We take $E_R(\varepsilon) = \exp(-\varepsilon^2/2R^2)/\sqrt{2\pi R^2}$ or $= [\vartheta(\varepsilon + R) - \vartheta(\varepsilon - R)]/2R$ according to numerical convenience.

The quasiparticle spectra are characterized by a coherent quasiparticle peak at an energy $\varepsilon \simeq \xi(k)$ and by shadow resonances at energies $\varepsilon \simeq \xi(k-q^i)$, produced by the interaction with charge and spin fluctuations. The shadow peaks do not generally correspond to new poles in the electron Green function and are essentially incoherent, although they follow the dispersion of the shadow bands. Their intensity varies strongly with k and increases as $\xi(k-q^i)$ approaches the value $\xi(k)$. In particular at the hot spots, where $\xi(k) \simeq \xi(k-q^i) \simeq 0$ there is a suppression of the coherent spectral weight near the Fermi level due to the strong scattering. In Fig. 1, on the right panel, we plot the energy distribution curves obtained along the direction ΓM (from top to bottom). The quasiparticle peak moves from the left to the right towards the Fermi level as the momentum is increased. It interferes with a shadow resonance associated with q^c , which appears in the third to seventh curves. This resonance moves initially to the left and then to the right, approaching the Fermi level. The effect of spin fluctuations is visible only near the M point, where a broad resonance appears below the Fermi energy and is located at -200 meV at the M point in Fig. 1.

We also study the k-distribution of low-laying spectral weight $w_k = \tilde{A}_R(k, \varepsilon = 0)$. This distribution is more appropriate than the standard definition of the FS in terms of quasiparticles, $\xi(k) + \text{Re}\Sigma(k, \varepsilon = 0) = 0$, in the presence of incoherent spectral weight near the Fermi

level. Indeed, the transfer of the spectral weight from the main FS to the different branches of the shadow FS at $\xi(k-q^i) \simeq 0$ produces features which are characteristic of the interaction with charge and spin fluctuations and of their interplay. In particular the symmetric suppression of spectral weight near the M points of the BZ, which would be due to spin fluctuations alone, is modulated by charge fluctuations (Fig. 1, left panel). This is also the case for the (weak) hole pockets produced by spin fluctuations around the points $(\pm \pi/2, \pm \pi/2)$. The interference with the branches of the shadow FS due to charge fluctuations enhances these pockets around $\pm(\pi/2, \pi/2)$ and suppresses them around $\pm(\pi/2, -\pi/2)$ (Fig. 1, left panel). Experimental results on this issue are controversial. Strong shadow peaks in the diagonal directions, giving rise to hole pockets in the FS, have been reported in the literature [18,32], where other experiments found only weak (or even absent) features [16].

We point out that, because of the transfer of spectral weight to the shadow FS, the experimentally observed FS may be rather different from the quasiparticle FS. The observed evolution could, indeed, be associated with the change in the distribution of the low-laying spectral weight, without any dramatic change in the topology of the quasiparticle FS, as was instead suggested in Ref. [33].

We interpret the suppression of portions of the FS as the onset of a pseudogap regime in the underdoped region. We attribute the pseudogap formation to the strong pairing associated with the singular e-e effective interaction in the Cooper channel (see below, Eq. 5). According to the scenario discussed in Ref. [6] the local gap formation should stabilize the system against the true static charge ordering. The self-consistent interplay of the various effects should be considered within a more refined model.

III. CROSSOVER BETWEEN D- AND S-WAVE GAP PARAMETER

Recent ARPES experiments indicate a crossover between d-wave and s-wave symmetry of the superconducting gap parameter driven by the increasing doping [26,27]. In order to describe theoretically the change of the symmetry of the gap parameter in the presence of

an almost unchanged FS, the effective electron-electron (e-e) interaction has to be doping dependent. This is the case for the effective interaction which arises near the Stripe-QCP [5,6,11,34]. In a first approximation we consider the e-e effective interaction in the Cooper channel as a sum of the spin and charge fluctuation contributions coupled to fermions

$$\Gamma_{Cooper}(q,\Omega) = \Gamma_c(q,\Omega) - \Gamma_s(q,\Omega), \tag{5}$$

where Γ_c and Γ_s are defined in formula (1), which gives the effective e-e interaction in the particle-hole channel. Note that the spin fluctuations contribute with a different sign in the p-p and p-h channels.

In the under- and optimally doped region, the pairing is due to the interplay between critical charge fluctuations, providing in the small q limit an attraction in both d-wave and s-wave channels, and spin fluctuations providing attraction only in the d-wave channel, being repulsive in the s-wave channel. Indeed small q interactions couple mainly nearby states in momentum space which have the same sign of the $d_{x^2-y^2}$ -wave symmetry factor $(\cos k_x - \cos k_y)$, preserving the attractive nature of the interaction. We point out that the effective interaction mediated by charge fluctuations includes, besides the small q attraction, a residual repulsive term at large q, as it was shown in Refs. [5,28]. However in our calculation this repulsion is accounted for by the interaction mediated by spin fluctuation. When both are considered, the $d_{x^2-y^2}$ -wave gap parameter is enhanced by the cooperative effects of charge and spin fluctuations up to optimal doping [11].

In the overdoped region it is likely that the spin fluctuations are strongly reduced, as suggested by the decrease of the antiferromagnetic correlation length at high doping [35]. In this region of the phase diagram the charge fluctuations are dominant and the gap parameter may be s- or d-wave, depending on the strength of the residual repulsion in the effective interaction. This crossover appears as a possibility in our model and indeed may or may not occur depending on the values of the parameters of the effective interaction as a function of doping. A dominant role of spin degrees of freedom at low doping and of charge degrees of freedom at higher doping in the pairing mechanism was also proposed in Ref. [36] in the

context of the three-band t-J-V model.

As shown in Ref. [34] the variation with doping of the charge instability vector q^c is another possible mechanism to induce a symmetry crossover. When q^c is less or of the same order of $2k_{Fy}$ (around M points) the gap has a $d_{x^2-y^2}$ -wave symmetry, since the interaction is characterized by small transferred momenta, whereas for q^c substantially greater than $2k_{Fy}$ the gap has an anisotropic s-wave structure. In this last case the $d_{x^2-y^2}$ -wave gap is strongly depressed because the large q interaction couples states with opposite sign of the corresponding symmetry factor, changing the attractive contribution into a repulsive one. In the cuprates these two mechanisms could coexist.

In the overdoped region, where we assume that κ_s^2 is sufficiently large, the q dependence of the effective interaction in the spin channel introduces minor correction with respect to the dominant term $\Gamma_s(q=q^s,\Omega=0)$. The relevant contribution of Γ_s to the effective interaction (5) is given by

$$\Gamma_s(q,\Omega) \simeq \Gamma_s(q^s,0) = -\frac{V_s}{\kappa_s^2} = -U.$$
 (6)

Thus, to simplify the discussion, we use in the following an effective interaction

$$\Gamma_{Cooper}(q,\Omega) = U + \Gamma_c(q,\Omega). \tag{7}$$

Within this approximation the contribution of the spin channel to the effective interaction (5) has the same effects as a residual repulsive interaction in the charge channel. In order to evaluate the symmetry and the momentum dependence of the superconducting gap, we consider the static part of the effective interaction given by $\Gamma(q) = \Gamma_{Cooper}(q, \Omega = 0)$, and we solve the BCS equation for the gap parameter $\Delta(k)$. The numerical value of the gap, obtained in the BCS approach, is only indicative because it is influenced by strong-coupling self-energy and non-adiabatic vertex corrections which have to be included in a complete generalized Eliashberg approach [37]. The BCS equation is given by

$$\Delta(k) = -\frac{1}{N} \sum_{p_x, p_y} \Gamma(k - p) \frac{\tanh \frac{\varepsilon(p)}{2T}}{2\varepsilon(p)} \Delta(p), \tag{8}$$

where $\varepsilon(p) = \sqrt{\xi^2(p) + \Delta(p)^2}$, and the bare electron dispersion $\xi(p)$ is a tight binding fit of the $Bi2212\ FS$ measured by ARPES at optimum doping [38]. The BCS equation is numerically solved taking advantage of the fast Fourier transform, as explained in Ref. [34].

Due to the qualitative character of the following discussion, we choose here a direction for the characteristic wave-vector q^c which emphasizes the d- vs s-wave crossover, and we take $q^c = (0, \frac{\pi}{4})$ along the ΓM direction. We consider a small mass term $\kappa_c^2 = 0.1$, pushing the system into the Momentum Decoupling regime [39].

In Fig.2 we report the condensation energy per particle as a function of $\frac{V_c}{U}$ for fixed $V_c = 0.4 eV$ for both the d- and s-wave symmetry: for $\frac{V_c}{U} < 5$ (up to optimum doping) the superconducting ground state has $d_{x^2-y^2}$ -wave symmetry while for $\frac{V_c}{U} > 5$ (which should correspond to the overdoped case) the symmetry is s-wave.

The s-wave gap parameter, obtained for small values of U, i.e. large doping, has an anisotropic momentum dependence along the FS (Fig.3). The s-wave gap parameter, normalized to its maximum value Δ_{max} , is plotted as a function of the angle ϕ which specifies the position of the Fermi momentum k_F on the FS with respect to the center of the closed FS for holes, which is located at the point $Y=(\pi,\pi)$. The anisotropic ratio $r=\Delta_{max}/\Delta_{min}$ is a function of U, at fixed $\kappa_c^2=0.1$ and $q^c=(0,\frac{\pi}{4})$. We find r=16.8 for U=0.12eV, r=2.4 for $U=U^*=0.08eV$ (where U^* is the crossover value between d- and s-wave symmetry) and r=1.68 for U=0.04eV giving a decreasing anisotropy for decreasing U, which corresponds to increasing doping, in agreement with the trend observed in ARPES experiments [26,27]. Notice, however, that from Fig.2, the transition from d- to s-wave superconductivity occurs at a $U/V_c \simeq 0.2$ ratio, where the anisotropy ratio $r \simeq 2.4$ is rather small. Therefore, at least for the (reasonable) parameters considered here, the d- to s-wave transition would be characterized by a rather abrupt decrease of anisotropy. This expectation could be tested experimentally by a detailed ARPES analysis at closely spaced fillings.

IV. CONCLUSIONS

In this paper we have briefly described the Stripe-QCP scenario and reported some of its consequences in the normal and superconducting states. Coming from the high doping regime, the occurrence of a charge-ordering instability towards a stripe phase, which is masked by the onset of a superconducting phase, provides the mechanism which controls the physics of the cuprates. It gives rise to the non-Fermi liquid properties of the normal phase, to some features found in ARPES experiments, and to the strong pairing interaction leading to d-wave superconductivity.

The main additional results of this paper concern the shape of the Fermi surface in the proximity of the Stripe-QCP and the symmetry of the superconducting gap, in comparison with the ARPES experiments on optimally [18] and over- doped Bi2212 [26,27].

By considering in our model a diagonal charge instability vector $q^c = (0.4\pi; -0.4\pi)$, as suggested by the experiments [18], we reproduce the asymmetrical spectral weight suppression around the M points observed in the normal state. We also describe the occurrence of shadow resonances in the energy distribution curves, which appear in addition to the quasiparticle peaks as a result of the interaction of the fermions with charge and spin quasicritical fluctuations.

In the superconducting state we obtain a $d_{x^2-y^2}$ -wave gap parameter in a wide range of parameters and we show that, within our scenario, it is possible to produce a d- vs s-wave gap symmetry crossover, and a reduction of the anisotropy of the s-wave gap with increasing doping, depending on the evolution of the parameters entering the effective interaction, as a function of doping. The main mechanisms which stabilize the anisotropic s-wave gap parameter, leading to the symmetry crossover, are the reduction of the residual repulsion and/or the increase of the charge instability vector q^c upon doping. A similar crossover was recently reported in ARPES experiments on overdoped Bi2212 [26,27]. Further experimental investigations are required to confirm a doping dependent crossover and to have a feedback on the theory.

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Fig. 1 LEFT: k-space distribution of low-laying spectral weight. The relative intensity decreases by a factor of two as the size of the black square is reduced. The energy resolution is taken R=25 meV, and the temperature is T=30 meV to compare with the results in Ref. [18]. The values of the other parameters are given in the text. RIGHT: Energy distribution curves along the ΓM direction for uniformly increased wave-vector k. The resolution is taken R=10 meV, and the temperature is T=10 meV, to compare with the results in Ref. [16].

Fig. 2 Condensation energy per particle for $V_c = 0.4eV$ and increasing U: d-wave (full line); s-wave (dashed line). The d-wave free energy is independent of U, because the momentum-independent repulsive contribution vanishes in the d-wave channel. According to our discussion an increasing V_c/U corresponds to increasing doping.

Fig. 3 Normalized s-wave gap for vertical direction with $q_y^c = \frac{\pi}{4}$ and decreasing values of $\frac{U}{V_c} = 0.3$ (dotted); 0.2 (short dashed); 0.1 (long dashed); 0.0 (full line).

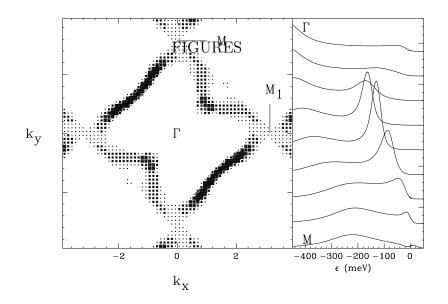


FIG. 1. S. Caprara et al.

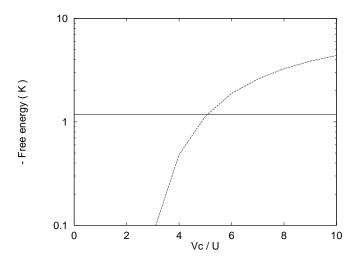


FIG. 2. S. Caprara et al.

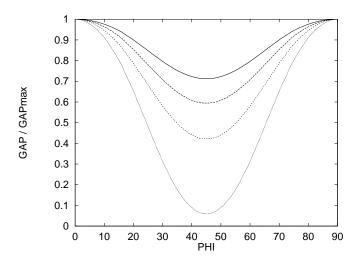


FIG. 3. S. Caprara et al.